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Diffusion in Stationary and Moving Grain Boundaries in Alloys

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Solutes in alloys can strongly interact with grain boundaries (GBs) and change their thermodynamic and kinetic properties. While it is well-established that solutes diffuse along GBs much faster than in the perfect lattice, understanding of this “short-circuit” diffusion phenomenon remain rather incomplete. This talk will address two topics related to GB diffusion: the effect of GB segregation on the diffusion rate, and the role of GB diffusion in the solute drag phenomenon. Both effects are studied by atomistic computer simulations combining molecular dynamics, Monte Carlo methods, and other computational approaches. The results demonstrate that solute segregation can cause either acceleration or retardation of GB diffusion, depending on the thermodynamics of the system, GB structure, and the segregation mechanism. While uniform segregation can accelerate diffusion in some systems, non-uniform segregation in the form of 2D nano-clusters (islands) causes strong retardation via the trapping effect. Both effects are different in high-angle and low-angle GBs, the latter case being dominated by dislocation pipe diffusion. In the solute-drag study, the drag force has been investigated systematically as a function of temperature, alloy composition, and the GB velocity. It is shown that solute diffusion along the GB can have a dramatic impact on the GB mobility by redistributing the solute atoms non-uniformly in the form of nano-clusters or islands, which then cause additional pinning of the boundary. It is known that the solute drag is controlled by solute diffusion across the moving boundary, but the role of diffusion along the boundary has not been appreciated before. Other interesting diffusion-segregation effects are also discussed.